

The NIH 3D Print Exchange: Whirlwind First Year

(Lessons learned from *naïve* Drupal users)

Capital Camp & Gov Days

July 31, 2014

Darrell Hurt, Ph.D.

Computational Biologist, Project Lead, NIH 3D Print Exchange
Bioinformatics and Computational Biosciences Branch
Office of Cyber Infrastructure and Computational Biology
National Institute of Allergy and Infectious Diseases



NIH 3D PRINT EXCHANGE



Discover



Share



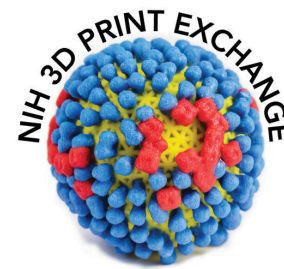
Create



Learn



Engage



Not Your Average (Government) Drupal Site



Autogenerates
custom 3D content



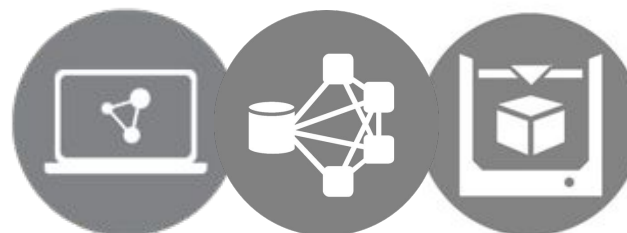
3D visualization
without modules or
plug-ins



Populates metadata
via XML



A little about me



Tram Huyen, Ph.D.
Branch Chief



Nick Weber, M.S.
Project Manager



Meghan Coakley, Ph.D.
Scientific Program Analyst



Makazi Mtingwa, A.L.M.
Drupal Developer



Jeremy Swan
Biovisualization Specialist



Seva Vsevelod
Software Developer



Meti Gizaw
Cyber Security Specialist



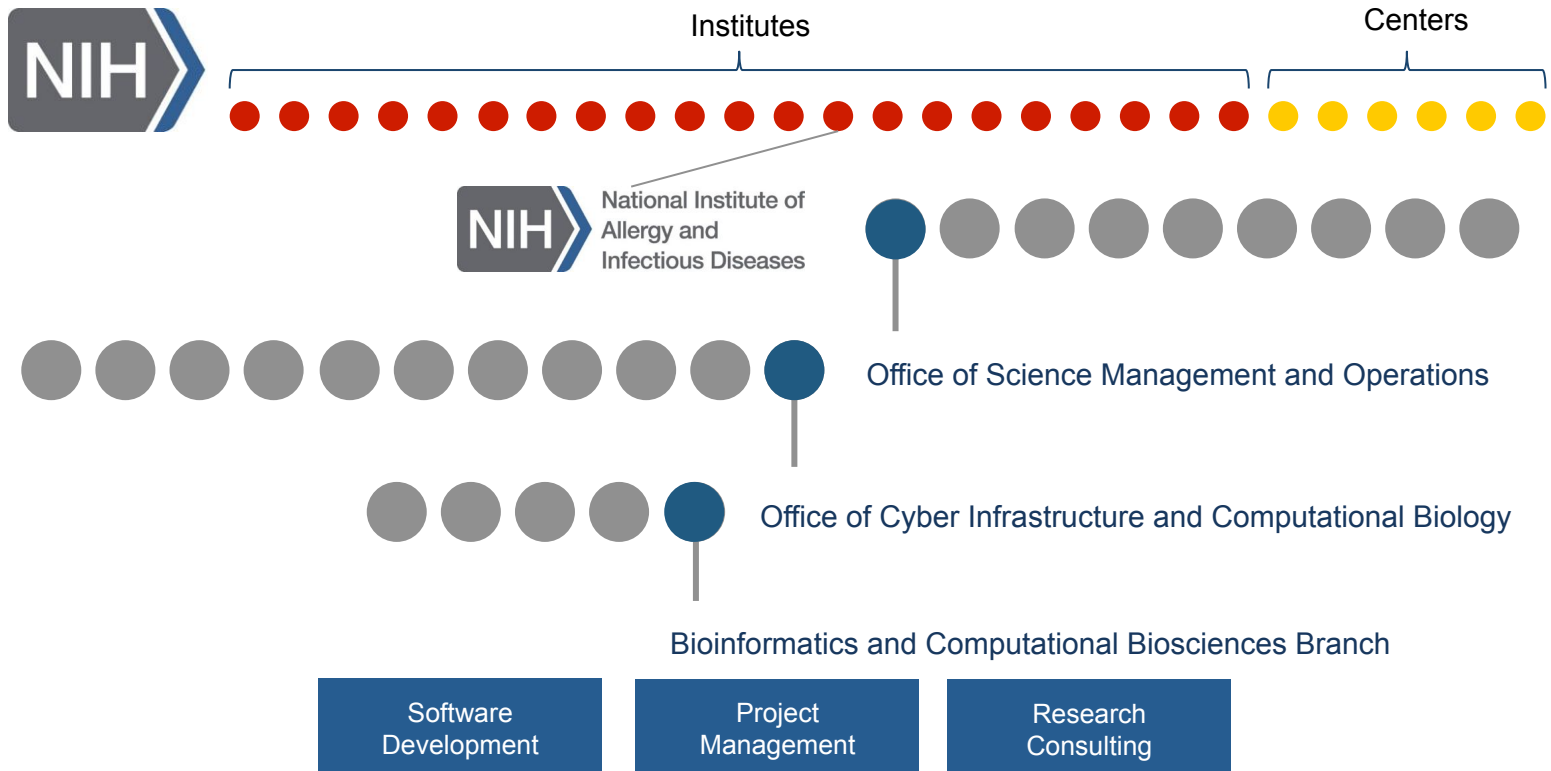
Alvin Yun
Linux Administrator



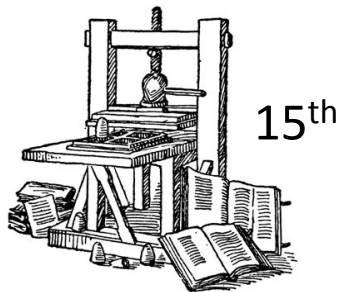
Erin Fincher
Scientific Illustrator



David Chen, Ph.D.
Biomedical Visualization



“3D printing has the potential to revolutionize the way we make almost everything.”



“3D Printing is this century’s most disruptive innovation.”

-David F. Flanders, TEDxHamburg, June 2011



Design a digital 3D image



Print layers



Enjoy your 3D object!



Tools and
household



Medical
implants



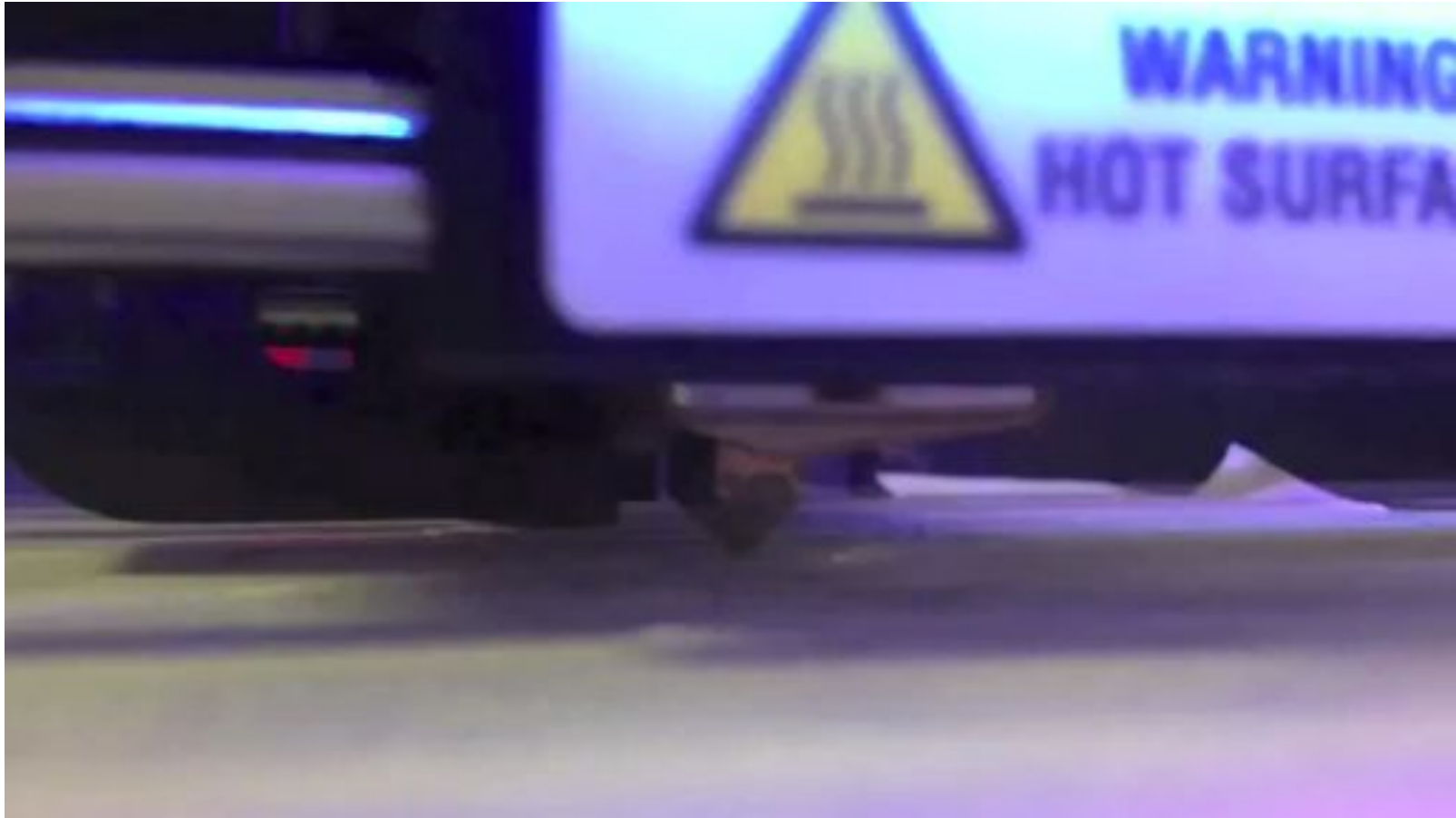
Educational
models

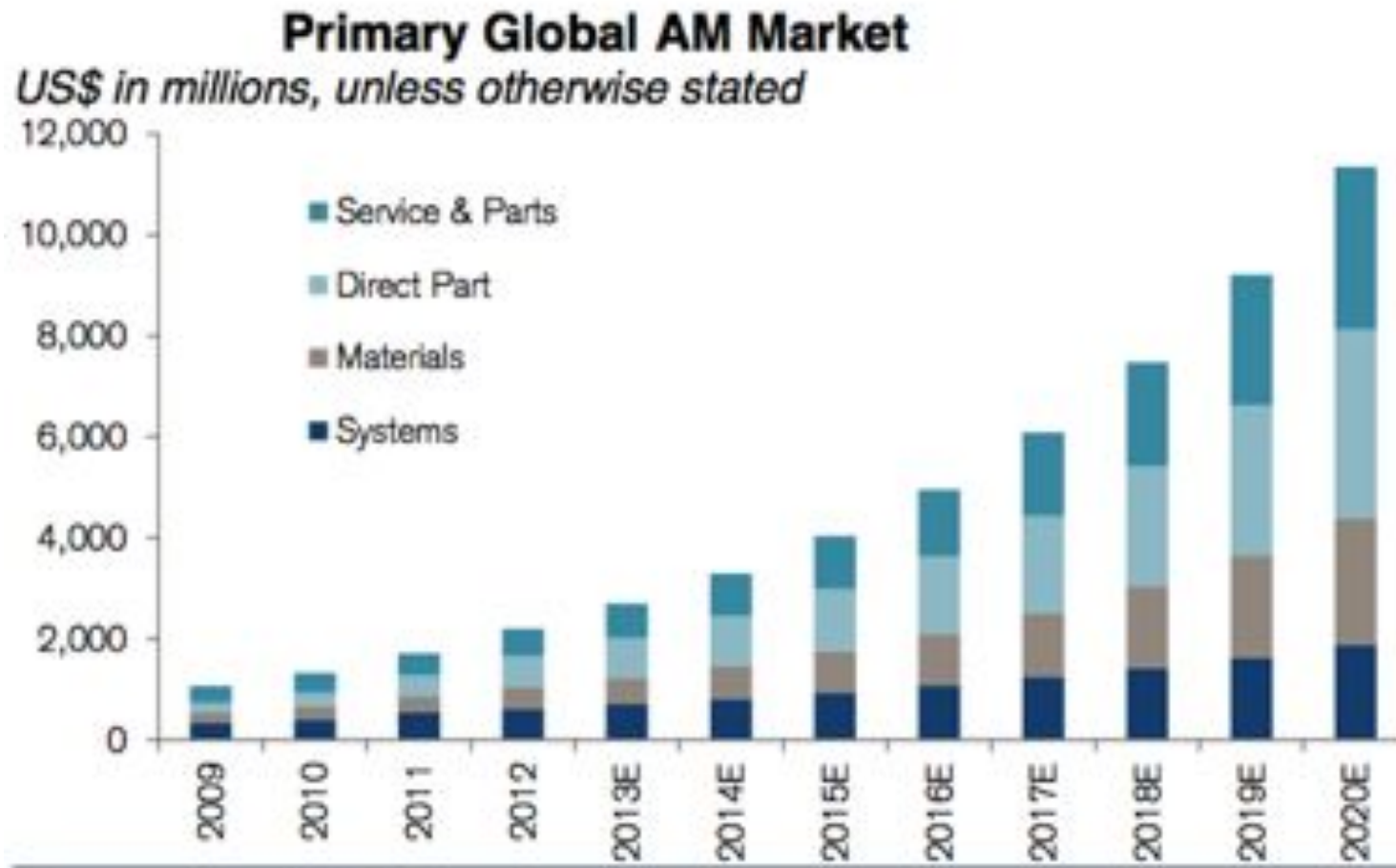


Toys and
gadgets



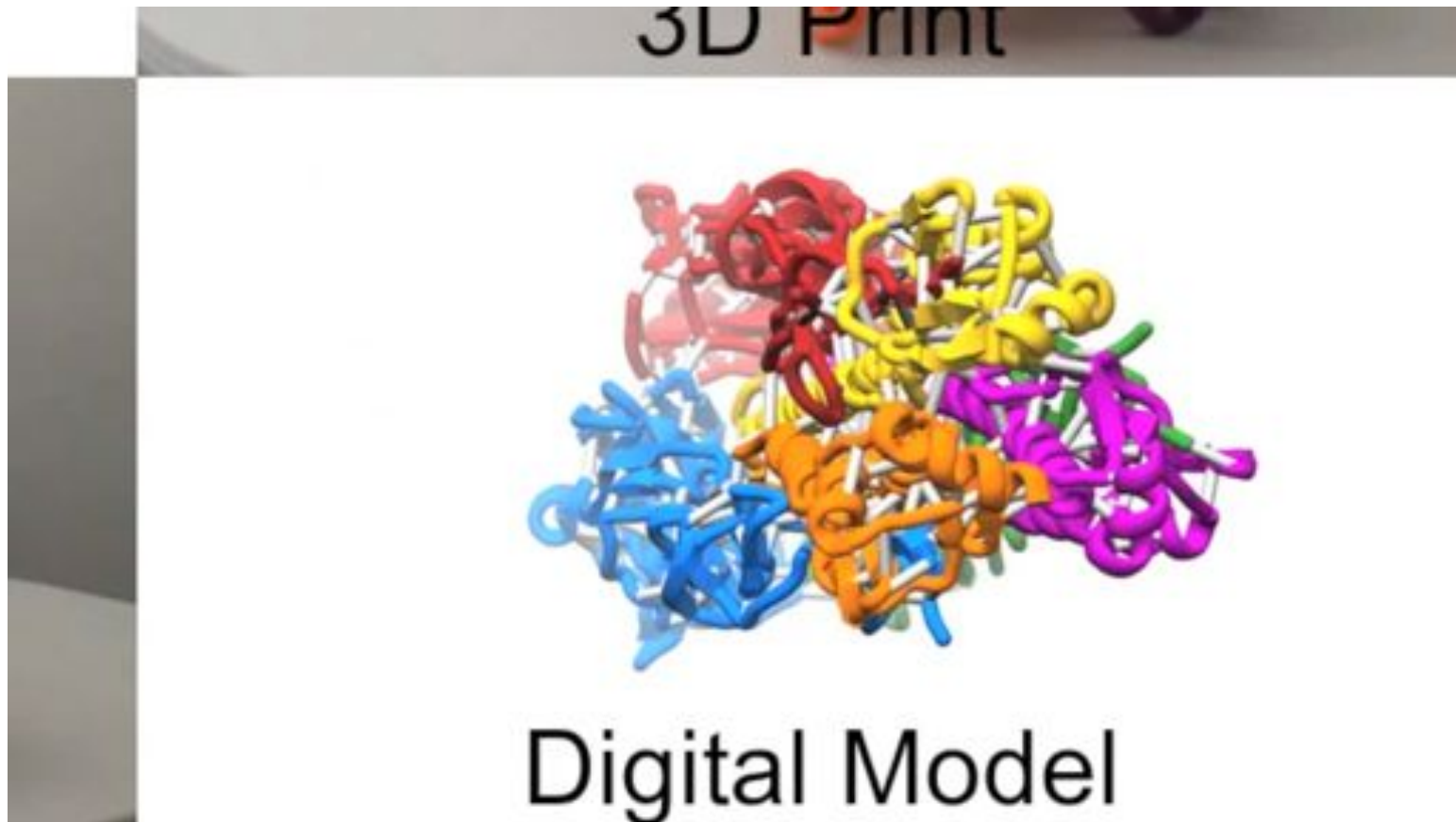
Shoes and
fashion





Source: Credit Suisse estimates.

How NIH uses 3D printing



3D models and prints are valuable, but difficult to create



Bryan Sivak
Chief Technology Officer, DHHS



HHS Ignite

Incubating New Ideas

August 2013 – February 2014



HHS Ventures

Accelerating Proven Concepts

June 2014 – March 2015

A community-driven resource for open data sharing

Click an image below to share your 3D-printable model



MEDICAL &
ANATOMICAL



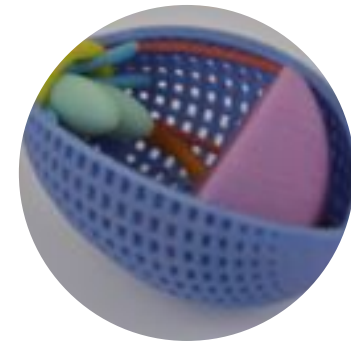
CUSTOM LABWARE



PROTEINS,
MACROMOLECULES,
& VIRUSES



BACTERIA,
ORGANELLES, CELLS,
& MORE



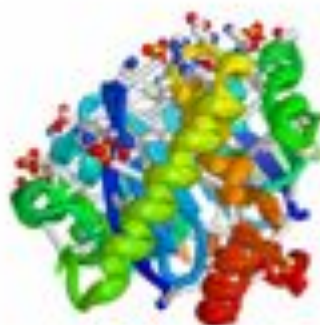
Novel, open source web tools save money
and maximize access



Click an image below to submit a data file.



MEDICAL IMAGING



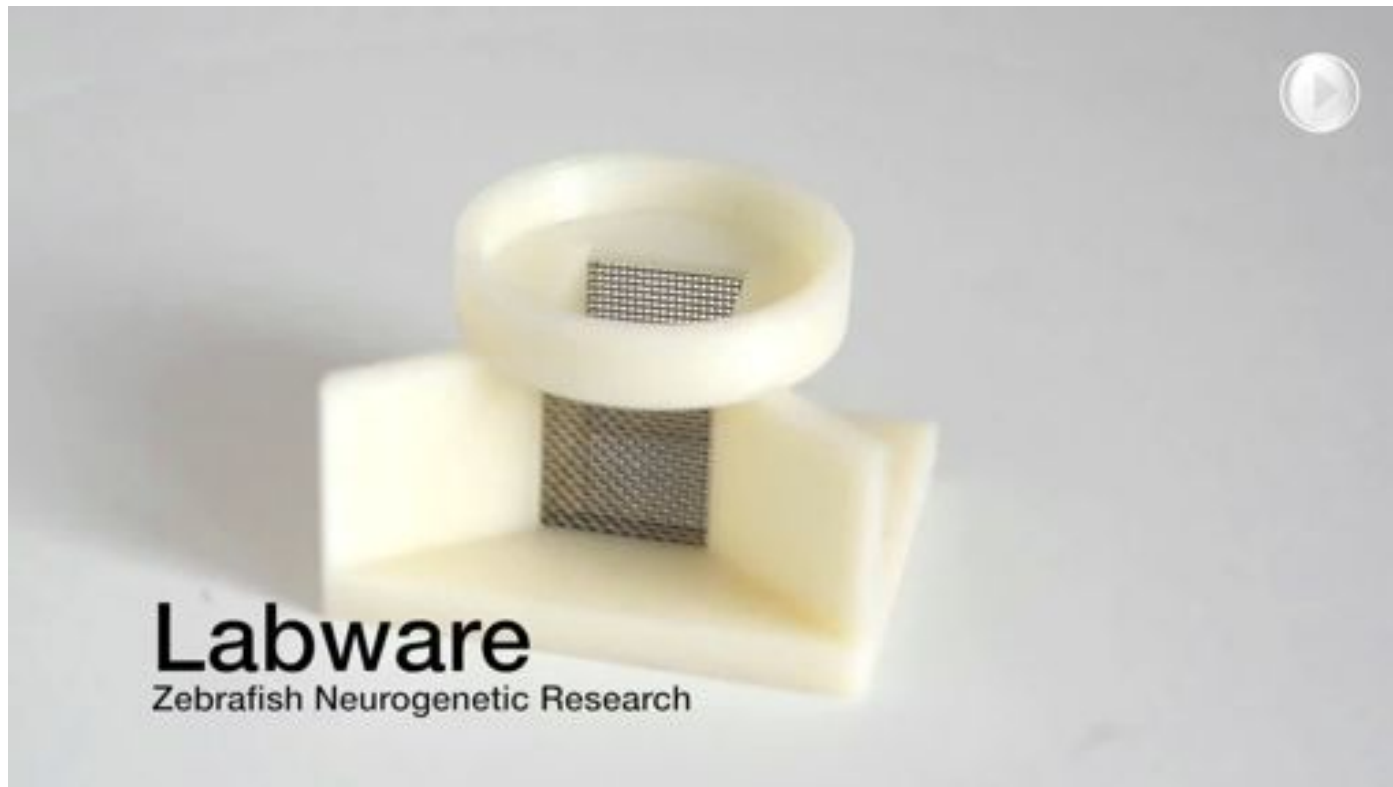
MOLECULAR DATA



IMAGE STACKS



Scientific Discovery





Physician and Patient Education





Hands-on Learning



How to develop a public government website in 12 months

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Research

Why we chose Drupal



- ✓ ☐ Open source
- ✓ ☐ Easy to implement
- ✓ ☐ Flexible
- ✓ ☐ Reputation
- ✓ ☐ Government “approved”



Lesson #1: The learning curve

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Research



OpenPublic



- Accessibility
- Security
- Base themes are responsive design-ready

Computational
Biology



Software
Development



Project
Management



Communications,
Neuroscience



Scientific Illustration,
Graphic Design



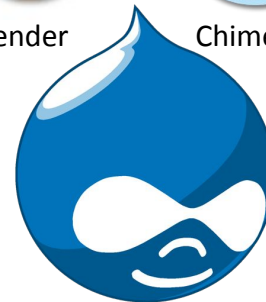
Blender



Chimera



Meshlab



Then we met the NIH Library folks. . .
. . .and started from scratch



Lesson #2: Collaborate & Iterate

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Research



OpenPublic

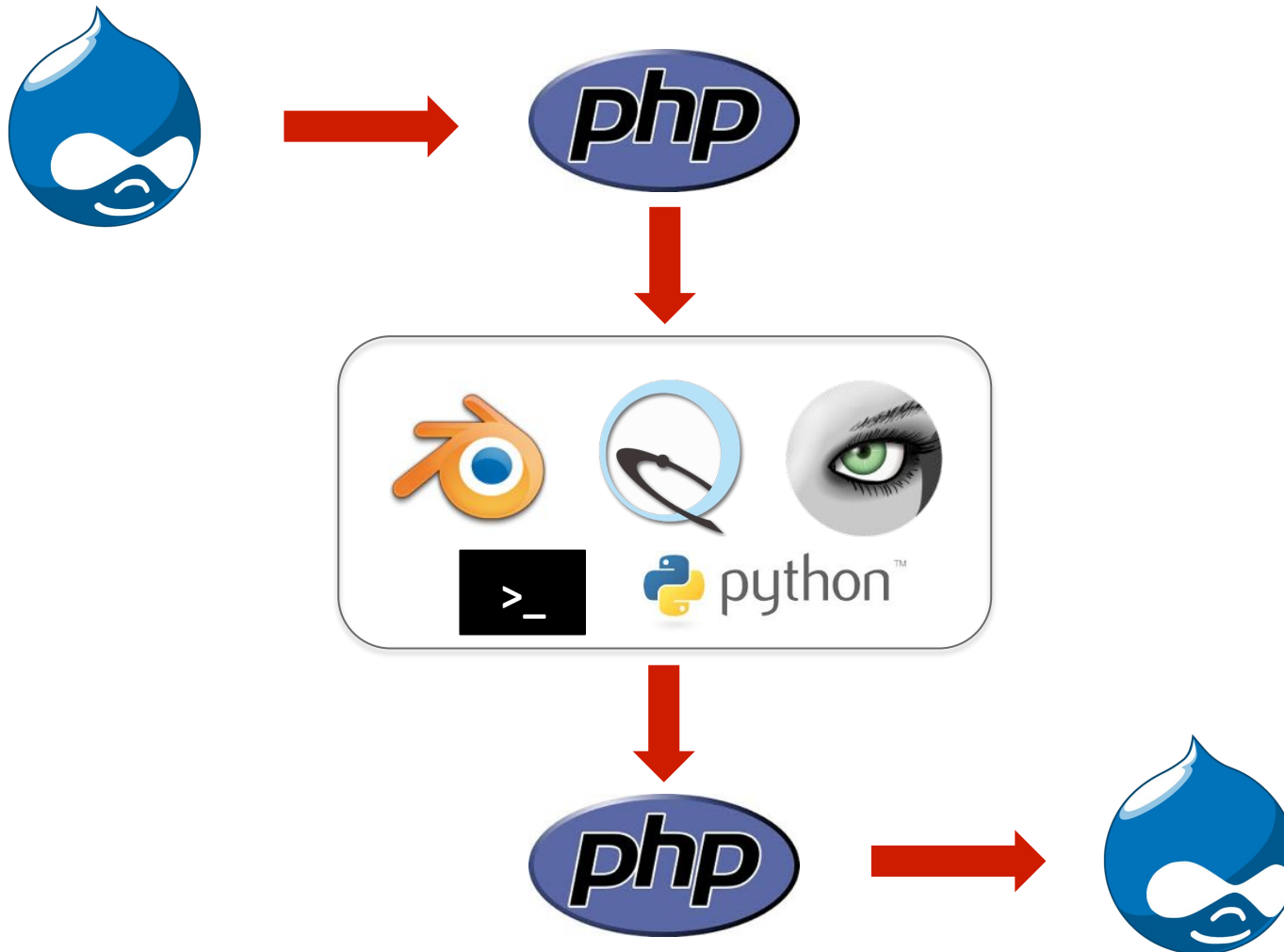


Acquia



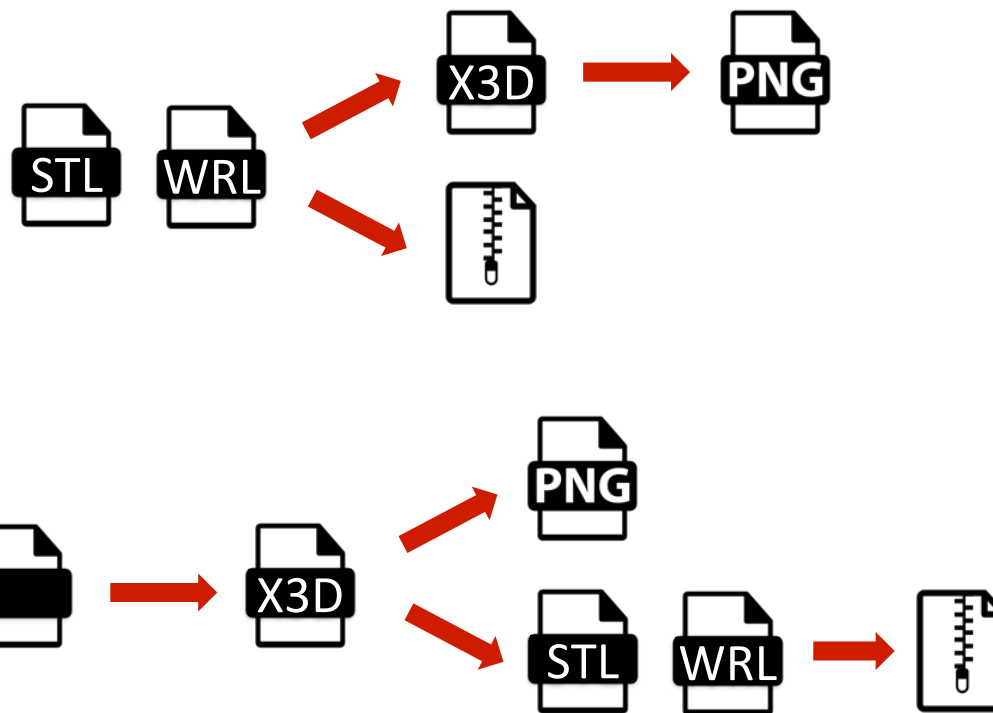
- Open source
- Practiced with local install
- Recommended by NIH Library
- Some help from Acquia consultants







Automated tools create 2D and 3D files



1

Crack Cocaine through DMs
Using an acid-catalyzed reaction

2

3

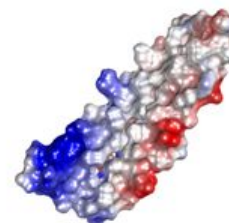
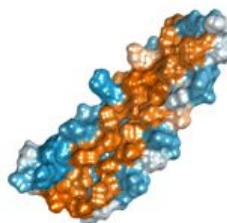
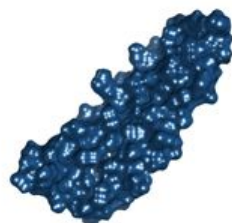
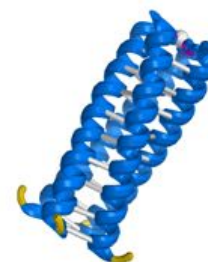
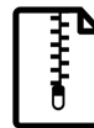
8

9

Colors such
as red, orange, yellow, green, blue, and purple



Colors by Kyle Ouellet, Hydrophobic (2008 Hydrophobic)





3D files need metadata!

PDB ID *

EMDB ID *

Submit *Enter a PDB or EMD* Submit

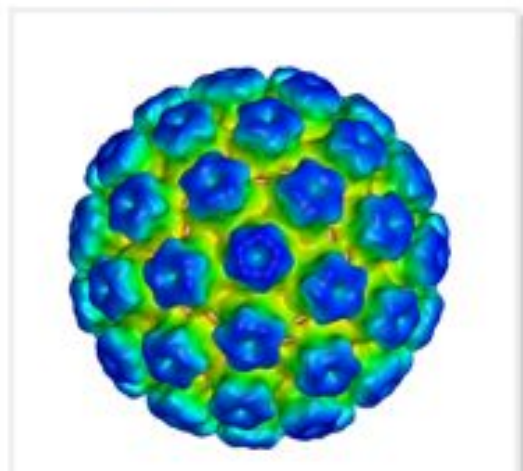
database accession number to generate a 3D-printable model of the structure.
(See instructions)

<http://www.ebi.ac.uk/pdbe/entry/EMD-5839/>

ftp://ftp.ebi.ac.uk/pub/databases/emdb/structures/EMD-5839/header/emd-5839.xml

Characterization of Human Papilloma Virus Type 16 VLP <title>

Submitted by:  3Dprint@NIH / Nov. 2014-07-16 18:30



MODEL DETAILS GENERAL INFORMATION
ATTRIBUTION

PubMed ID [24,299,977](#)

<external reference type="pubmed">

Digital Object Identifier (DOI)
[10.4161/hv.27316](#)

<external reference type="doi">

Author(s)

Zhao Q, Potter CS, Carragher B, Lander G, Sworen J, Toene V, Abraham D, Duncan P, Washabaugh MW, Sitrin RD

<authors>

Citation Title

Characterization of Virus-Like Particles in GARDASIL by Cryo Transmission Electron Microscopy

<articleTitle>

Citation Year 2013

<year>



U.S. Department of Health and Human Services — National Institutes of Health

NIH NIH 3D Print Exchange

DISCOVER SHARE CREATE LEARN ENGAGE NEWS & EVENTS ABOUT SEARCH

Search Terms:

Category:










Color: ☒ Monochrome ☐ Multicolor ☐ Full Spectrum

License:

For Education? ☒ Any ☐ No ☐ Yes

Sort by:

Order:

<p>Lumbar Spine - L2 fracture</p> 	<p>Lumbar Spine - fracture</p> 	<p>Lumbar Spine - Mega Apophysis</p> 
		
<p>3DPX-000405</p> <p>Radio and Ultra</p> 	<p>3DPX-000404</p> <p>Cervical Spine</p> 	<p>3DPX-000403</p> <p>Shoulder Fracture - Proximal Humerus</p> 

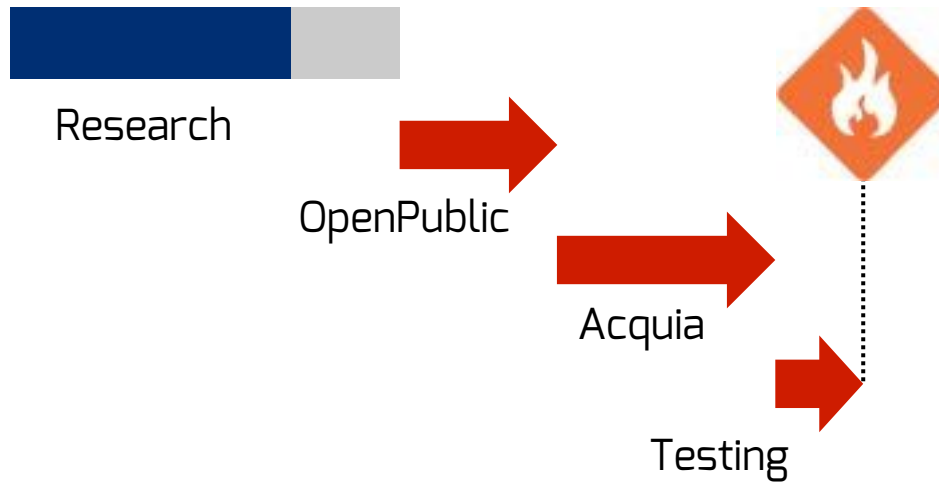


Lesson #3: Break ALL the rules

“Private” beta testing

- Temporary ATO to allow public access
- Small test group of advisors, collaborators, and invited contributors
- Available only if you know the “password”
shhhh! It’s “/acquia”

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HHS Shark Tank February 7, 2014

Mark Rohrbough
Director, Center for Technology Transfer
National Institutes of Health (NIH)

Taha Kass-Hout
Chief Health Information Officer
Food & Drug Administration (FDA)



We were on the right track, but still a long way to go. . .

. . .so we called in a (Drupal) professional



Makazi Mtingwa, A.L.M.
Drupal Developer

- Drupal, PHP
- Graphic design
- 3D animation (!)

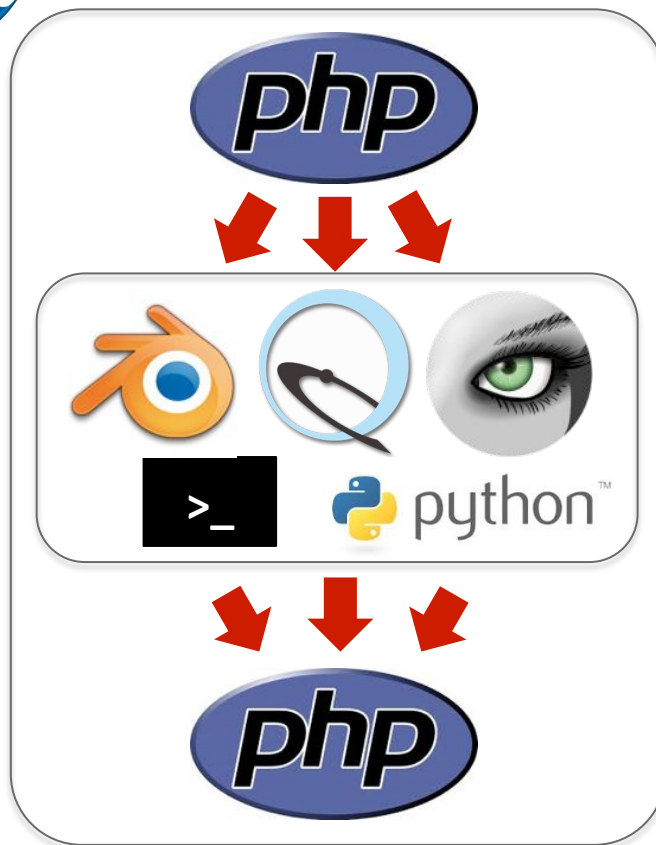
“What is going on here?”

- Five different custom content types for models
- Too many modules
- No version control
- Numerous HTML “hacks”
- Clunky CSS
- No custom page templates

“Uh, that’s the only way **we**
could get it to work”

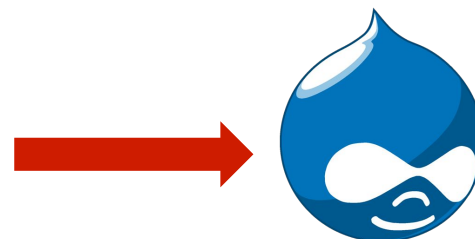


Lesson #4: Less is more



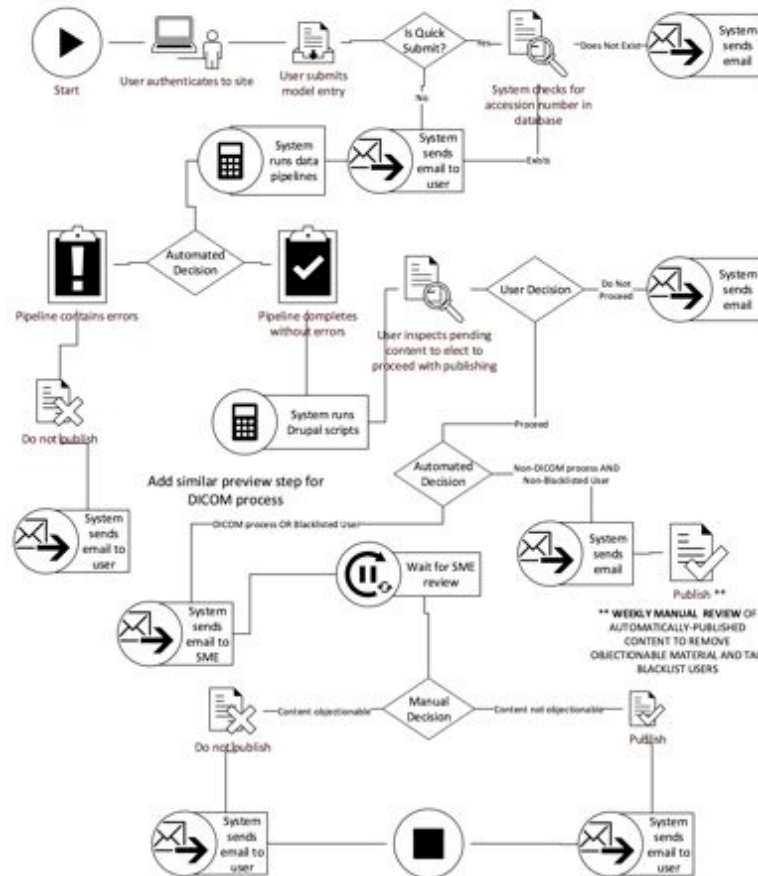
Custom Module

- Creates 10 different forms from 30+ field custom content type
 - Eliminates need for conditional fields
- Bootstraps Drupal to run in background & uses queueing
- Publishing workflows



Custom Module

- Publishing workflows
 - Provides privacy & protection



Custom Theme

The screenshot displays the NIH 3D Print Exchange website with a custom theme for the protein Estradiol 17 Beta-Dehydrogenase 4, Oxtoxynol-10. The page features a dark header with the NIH logo and navigation links. The main content area includes a large 3D molecular model of the protein, a sidebar with a search bar and a 'SHARE' button, and a footer with a 'Log in' button. The custom theme is highlighted by a red border around the main content area, which includes a 'DISCOVER' section with a 'Find 3D model' button and a 'CARTOO' section with a 'Cartoon of 3D model' button. The main content area also displays the protein name, a 3D model, and a list of related models.

NIH 3D Print Exchange

ESTRADIOL 17 BETA-DEHYDROGENASE 4, OXTOXYNOL-10

DISCOVER

Find 3D model

Home - Cart

CARTOO

Cartoon of 3D model

http://www.nih.gov/3dprintexchange

Content creator

3D

Model ID: 3DPEX-000000

Category: Proteins, Macromolecules and Molecules

Protein Data Bank ID: 3JL2

Model Color: Full spectrum color

Monochrome

Log in

SHARE

Search

OUT


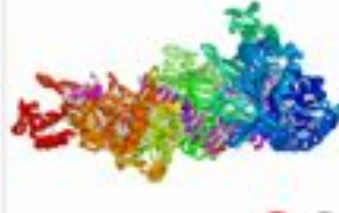



Information

Bill Hert

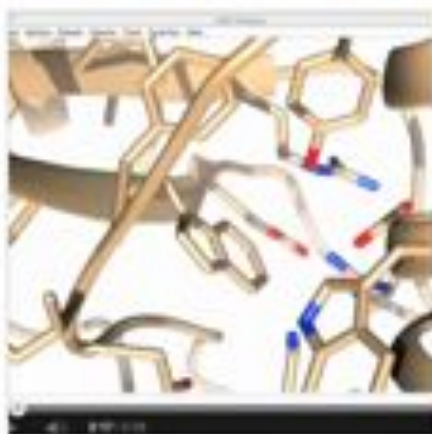
Additional Improvements

- Better file system structure
- Automatic uploads for large data (Javascript)
- Link buildographies to model pages
- Responsive design potential
 - Eliminated tables
 - Blocks with CSS

Recently Added Models

			
<p>3DPX-000486</p> <p>5'- D(*DA*DCP*DAP*DCP*DT P*DAP*DCP*DAP*...</p> <p> Meghan Coakley</p>	<p>3DPX-000485</p> <p>PROTEIN recA/DNA Complex</p> <p>christopher.fer...</p>	<p>3DPX-000484</p> <p>Troponin C/Troponin T/Troponin I</p> <p>christopher.fer...</p>	<p>3DPX-000483</p> <p>ADAM 22</p> <p>christopher fer...</p>

Tutorials



Mutating a Residue in UCSF...



Darrell Hurt

Thu, May 28, 2014 05:05 pm

This video demonstrates how to create a mutation in UCSF Chimera and to...

Chimera, tutorial, mutation, residue, UCSF



Mutating a Residue in UCSF...

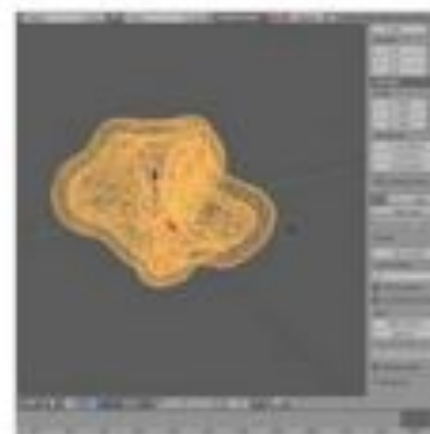


Darrell Hurt

Thu, May 28, 2014 05:05 pm

This video demonstrates how to make a mutation and accommodate said muta...

Chimera, tutorial, UCSF, mutation



Hollowing out a 3D Model for...



Darrell Hurt

Tue, May 27, 2014 01:05 pm

You can save time, money, and materials by hollowing out 3D model files...

Chimera, tutorial, model

What's New



Capital Camp & Gov Days...



Nick Weber

Tue, July 29, 2014 07:07 pm

NIH 3D Print Exchange Team Lead, Dr.

outreach, research, conference, design, government



Recap: White House Maker Faire



Meghan Coakley

Tue, June 24, 2014 12:06 pm

Finally!

White House, Maker Faire, outreach



Official Site Launch



Meghan Coakley

Tue, June 19, 2014 12:06 pm

Houston, we have lift off!

site launch, White House, #nationofmakers, Maker Faire



- [Blog](#) (12)
- [Event](#) (7)
- [News](#) (4)

#nationofmakers

3D Printing Industry 3DPX ID attribution conference domains CNA drupal education exhibit festival genome government hackerspace HRS IDEA Lab ideospace keynote Maker Faire microscopy modeling neuroscience OSTP outreach publishing reviews site update smithsonian support symposium synapse tutorial

USASEF Ventures

White House

• JULY •

S	M	T	W	T	F	S
			1	2	3	4
5	6	7	8	9	10	11
12	13	14	15	16	17	18
19	20	21	22	23	24	25
26	27	28	29	30	31	

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Research



OpenPublic



Acquia



Testing



"Private" Beta





Lesson #5: Deadlines!



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Research



"Private" Beta

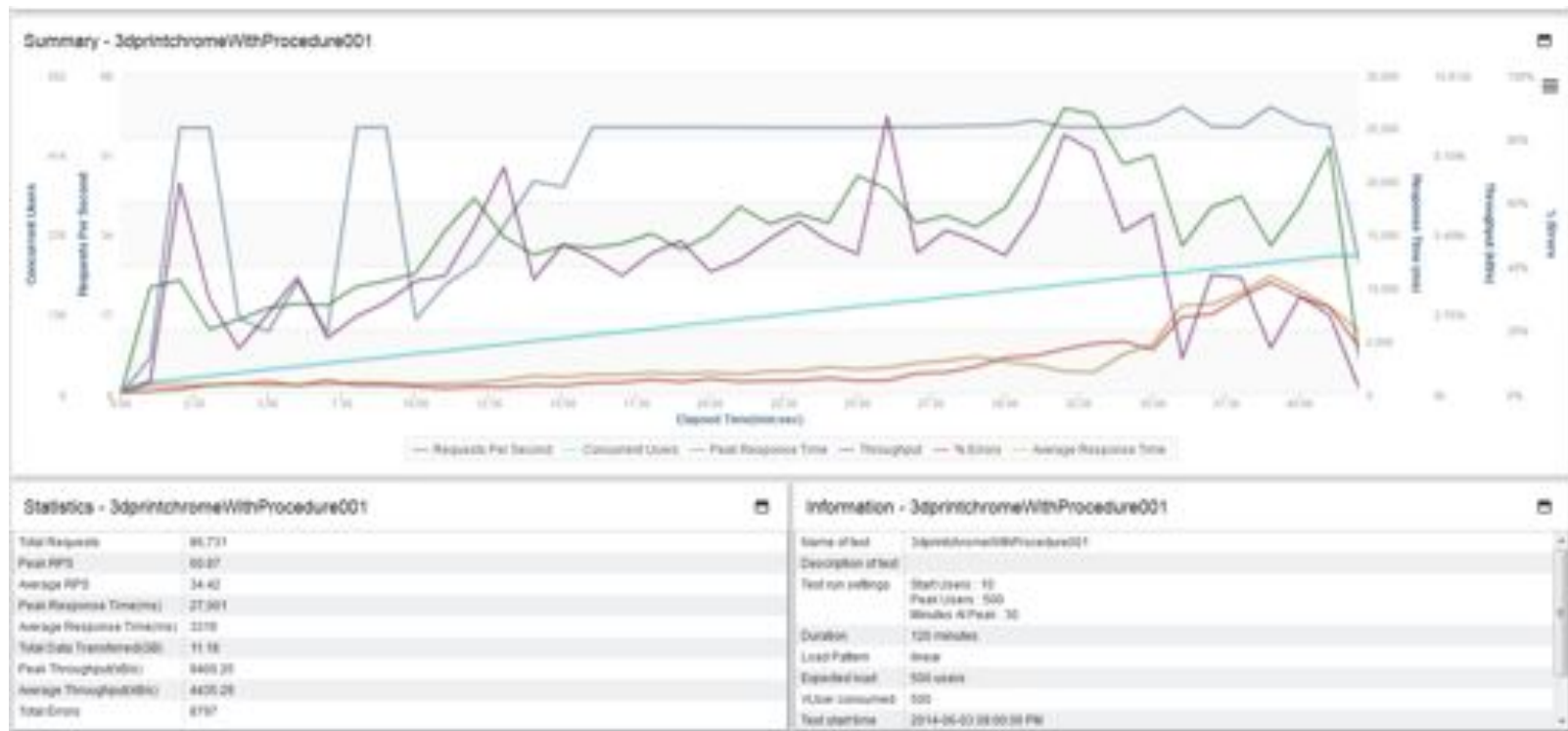


Public Beta

Performance Testing



! Test failed at 25 minutes, <60 concurrent users



Load-Handling Solutions

- Drupal caching system
- Memcache
- Varnish
- MySQL DB on separate server
- Increased CPU and memory



2,000 concurrent users and multiple data processing pipelines

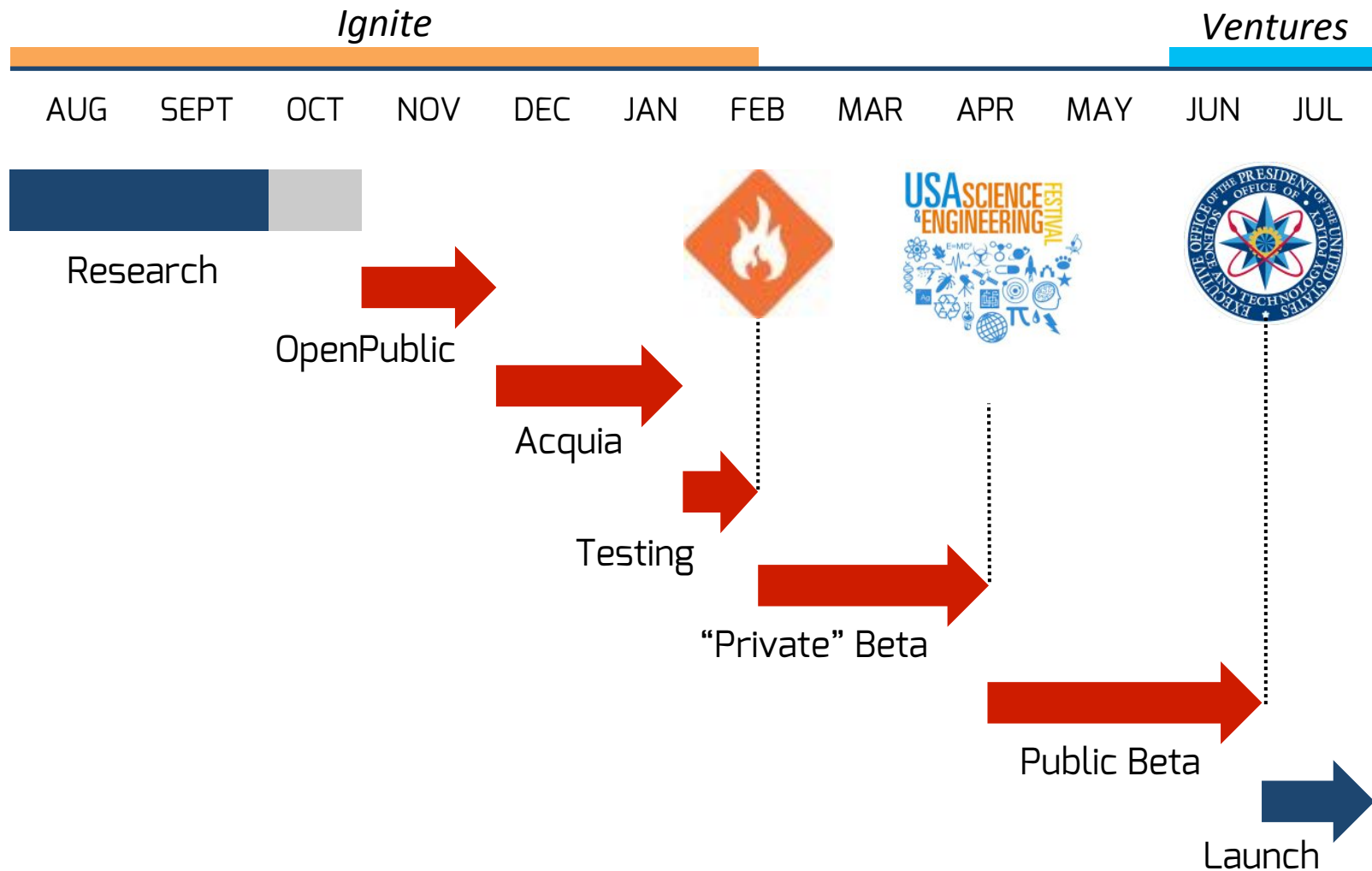


Server specifications



- Production web server
 - 4 vCPU (16 cores)
 - 18 GB memory
 - Separate dedicated production-level MySQL database server
 - Enterprise storage: 500 GB reserved (can grow as needed)
 - 90-day backup
- Dev & QA web servers
 - 2 vCPU (8 cores)
 - 12 GB memory
 - Integrated MySQL database
 - Integrated storage
 - No backup
- Version control server (Git)

Mini-lesson:
SVN doesn't work well
for Drupal
deployment





Lesson #6:
Cultivate user base,
seek “air cover”, and
align with greater initiatives

Janet Iwasa, Ph.D.

Louisa Stark, Ph.D.

Tim Herman, Ph.D.

David Hall, Ph.D.

Anthony Rotolo, Ph.D.

Capt. Gerald Grant, D.M.D.

Sharon Strauchs

Nicholas Polys, Ph.D.

George Phillips, Ph.D.

Graham Johnson, Ph.D.

Art Olson, Ph.D.

Tom Ferrin, Ph.D.

Outreach Events



September 27-28, 2013



November 6-8, 2013



Outreach Events



March 14, 2014



May 7, 2014



Outreach Events

May 22, 2014



Smithsonian
National Museum of Natural History



NMNH @NMNH - May 22
Join us in the #GenomeZone and help @NIH3Dprint build a DNA model!
@UnlockLifesCode pic.twitter.com/vs1DrvXebG



Expand

Reply Retweeted Favored More

Outreach Events



June 8-9, 2014



CONFABULATION
Symposium on 3D in the classroom

June 25, 2014



Capital Camp and Gov Days '14

Outreach Events

August 6-11, 2014



September 5-7, 2014



September 14, 2014

August 8-14, 2014



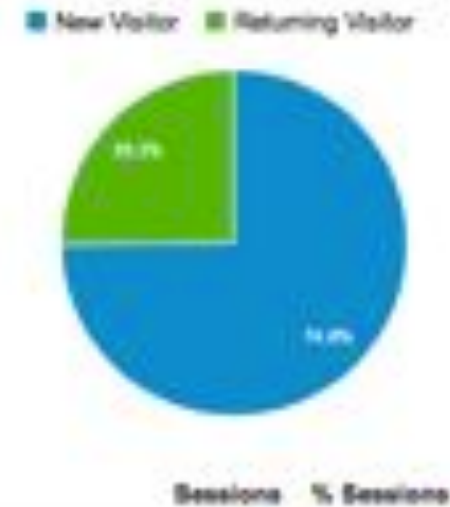
Official Launch: White House Maker Faire

June 18, 2014



“We hope that the 3D Print Exchange will expand interest and participation in this new and exciting field among scientists, educators and students.”

Dr. Francis Collins, Director, NIH





& 40+ professional blogs
and websites

Continued Improvement

- Build API for batch submission and download
- Faster content generation
- Better search features
- Faster 3D viewer
- Revisions, provenance, more metadata
- Move to public GitHub
- Repurpose framework and security documentation

Goal: Open Data & Open Science

- d) When available and where not limited by law, **make freely and easily accessible** to the public all digital files in the highest available fidelity and resolution, including, but not limited to, photographs, videos, and **digital 3D models**, and associated records and documentation, describing or characterizing objects in government-managed scientific collections.

Agencies should work together to share and coordinate policies, where appropriate, through the IWGSC.



March 20, 2014

Tom Kalil
Deputy Director for Policy
Office of Science and Technology Policy





<http://makezine.com/2014/03/29/toward-thingiverse-gov/>

3Dprint.nih.gov



3Dprint.nasa.gov

3Dprint.nist.gov

3Dprint.army.mil

3Dprint.???.gov

Open government is good

- Innovation flourishes when people have the freedom to experiment
- Good team makes the difference
- Open hardware
- Open software
- Open framework
- Open documentation
- Open data
- Open science
- Communication, collaboration, and transparency = community

Acknowledgements

NIAID

Anthony Fauci, M.D.
J.J. McGowan, Ph.D.
CIO Mike Tartakovsky
CTO Alex Rosenthal
Joe Croghan
James Ashton

NICHD

Jeremy Swan
Chandan Sastry, Ph.D.
Jennifer Lippencott-Schwartz, Ph.D.
Harold Burgess, Ph.D.

NLM

Michael Ackerman, Ph.D.
Terry Yoo, Ph.D.

NCATS

Eric Jones



DHHS

Deputy Secretary Bill Corr
Bryan Sivak
Read Holman
Will Yang
Damon Davis

NIH OD

Francis Collins, M.D., Ph.D.
Scott Prince
Marin Allen, Ph.D.

NIH Library

James King
Ben Hope
MaShana Davis

NIH CIT

Dan Luxenberg

Thank you!

Please visit our site – we welcome
your feedback!



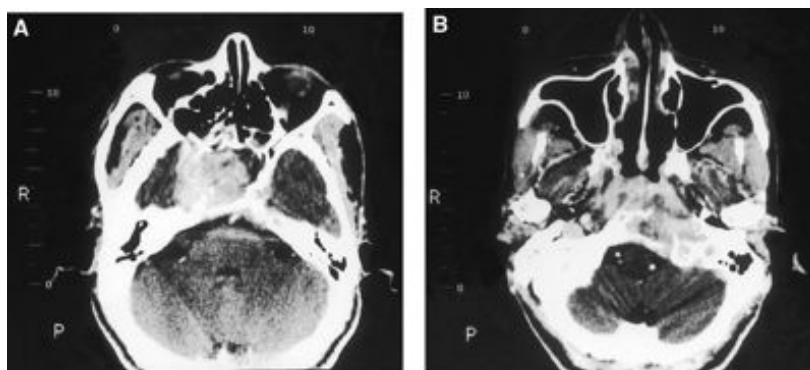
3Dprint@nih.gov



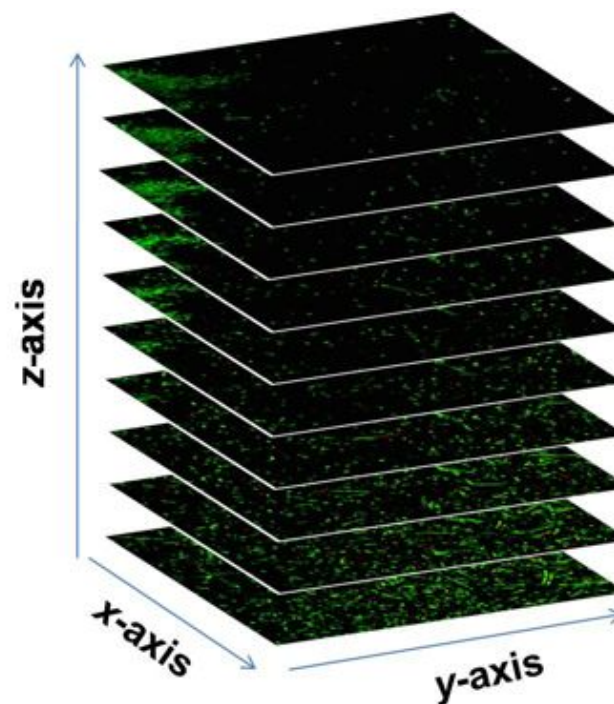
NIH 3D Print Exchange



@NIH3DPrint



ATOM	1	H	GLY	A	1	44.842	51.034	101.294	0.01	27.23
ATOM	2	CA	GLY	A	1	45.640	50.230	100.389	0.01	26.09
ATOM	3	C	GLY	A	1	44.692	49.640	101.300	0.01	26.00
ATOM	4	O	GLY	A	1	46.090	50.222	100.381	0.01	26.91
ATOM	5	H	SER	A	2	47.103	48.518	100.951	1.00	26.26
ATOM	6	CA	SER	A	2	48.177	47.845	101.741	1.00	26.17
ATOM	7	C	SER	A	2	49.212	47.031	100.945	1.00	24.21
ATOM	8	O	SER	A	2	49.040	47.195	99.430	1.00	19.77
ATOM	9	CB	SER	A	2	47.458	47.091	102.000	1.00	26.31
ATOM	10	OG	SER	A	2	44.176	44.356	102.404	1.00	27.00
ATOM	11	H	HIS	A	3	50.147	44.166	101.370	1.00	23.93
ATOM	12	CA	HIS	A	3	51.129	45.389	100.689	1.00	21.44
ATOM	13	C	HIS	A	3	50.953	43.905	100.049	1.00	20.32
ATOM	14	O	HIS	A	3	50.330	43.595	101.950	1.00	22.00
ATOM	15	CB	HIS	A	3	52.535	45.674	100.990	1.00	19.69
ATOM	16	CG	HIS	A	3	51.940	47.090	100.411	1.00	21.44
ATOM	17	HD1	HIS	A	3	53.371	47.470	99.402	1.00	20.07
ATOM	18	CB2	HIS	A	3	52.936	48.175	101.433	1.00	21.69
ATOM	19	CE1	HIS	A	3	52.476	48.730	99.474	1.00	20.57





IDTechEx 2014

Capital Camp and Gov Days '14